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CFD Analysis of Spatial Distribution of Various Parameters in Downdraft Gasifier

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Abstract

Gasification converts carbonaceous pulverized fuels into synthesis gas, a mixture of CO and H_2 that is a raw material for chemicals as well as a fuel for producing electricity. Gasification produces a much higher concentration of carbon dioxide than direct combustion of coal in air. In view of these, gasification energy combined with Computational Fluid Dynamics (CFD) software has been described in some detail in the following study. The aspect of gasification processes have been investigated for down-draft gasifier using simulation in FLUENT software. The formation of flow pattern, temperature, turbulence and product gas composition were investigated. Some of the results are compared with the results available from the literature.

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Keywords: CFD; Downdraft gasifier;Lignite gasification

Nomenclature

E	*Energy (J)*
$\vec{F}$	*Force applied (N)*
J	*Diffusion of species*
P	*Pressure (N/m^2)*
S	*Source term*
T	*Temperature (K)*
Y	*Mass fraction*
Z	*Mass fraction for element*
f	*Mole fraction*
$\vec{g}$	*Gravitational acceleration (m/s^2)*
h	*Enthalpy (J)*

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$\vec{v}$	*Velocity in the direction of (m/s)*
Greek symbols	
ρ	*Density of fluid (kg/m^3)*
λ	*Effective conductivity*
v	*Kinematic viscosity*
$\bar{\tau}$	*Shear stresses*
Subscripts	
m	*Mass*
eff	*Effective*
h	*Enthalpy*
j	*Species/Element*
s	*Species*

1. Introduction

Gasification of lignite converts solid particles into synthesis gas that can be used in a modern conversion device, such as gas turbines or engines, for electricity and heat production. It combines high efficiency even at a low scale and cost-effective reduction of pollutant emission. Many researchers carried out experimental and theoretical analysis and tried to find out relationship between results. Wang Yiqun and Yan Lifeng [1] gave Computational Fluid Dynamics (CFD) modeling applications on biomass thermo-chemical processes which help to optimize the design and operation of thermo-chemical reactors. Details of fundamentals for developing a CFD solution is described in paper. Baggio P., Baratieri M., Fiori L., Grigiante M., Avi D., Tosi P. [2] carried out experimental and modeling analysis of a batch gasification/pyrolysis reactor. The experimental results have been compared against calculations obtained by applying a thermo-chemical equilibrium model, improved to predict both the gas and the solid phase product yields. N.K.Ram, S. Maji and B.B.Arora [3] did simulation of down draft biomass gasification using CFD. Variation in gas composition and calorific value of the producer gas with varying equivalence ratio is checked in order to predict the performance of the downdraft gasifier. The present computational fluid dynamic models are unable to solve such complex reaction mechanisms due to its complexity. Brink et al. [4] created a model for biomass combustion using single-step mechanics and turbulence-chemistry interaction with eddy dissipation combustion model as the air distribution were injected around the bottom of the model. The same combustion model and turbulence model approach is used here.

2. Gasification Equations

In a gasifier, various chemical reactions take place inside the system. These reactions can be broadly divided into 2 categories i.e. Homogenous reaction and Non-homogenous (Heterogeneous) reactions:

Heterogeneous reactions

Reaction 1: Boudouard reaction:

$$C + CO_2 \Leftrightarrow 2CO \quad (1)$$

Reaction 2: Water gas (primary) reaction:

$$C + H_2O \Leftrightarrow CO + H_2 \quad (2)$$

Reaction 3: Methanation reaction:

$$C + 2H_2 \Leftrightarrow CH_4 \quad (3)$$

Reaction 4: Steam reforming reaction:

$$CH_4 + H_2O \Leftrightarrow CO + 3H_2 \quad (4)$$

Reaction 5: Water gas shift reaction:

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \quad (5)$$

Homogenous reactions

$$2H_2 + O_2 \rightarrow H_2O \quad (6)$$

$$CO_2 + H_2 \Leftrightarrow CO + H_2O \quad (7)$$

3. Modeling

The geometry of the gasifier created using GAMBIT 2.2.30 [5] is shown in Figure 1. The gasifier is divided into four regions: a combustion region near the throat, a reduction region above the combustion zone, oxidation zone above the

reduction zone and finally drying zone on the top of the gasifier. Air enters gasifier through three air tuyeres positioned at the top of the gasifier and aimed at the throat inside the gasifier. Lignite is already filled in the gasifier.

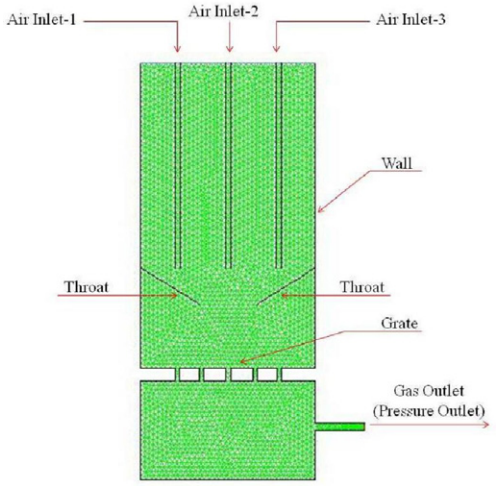

Fig. 1. Grid

3.1 Governing Equations

The equations for conservation of mass, conservation of momentum, and energy equation are given as:

$$\nabla \cdot (\rho \vec{v}) = S_m \tag{8}$$

$$\nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\bar{\tau}) + \rho \vec{g} + \vec{F} \tag{9}$$

$$\nabla \cdot (v(\rho E + p)) = \nabla \cdot (\lambda e_{ff} \nabla T - \sum h_j j_j + (\vec{\tau}_{eff} \cdot \vec{v})) + S_h \tag{10}$$

where, λ_{eff} is the effective conductivity (l+lt, where lt is the turbulence conductivity) and J_j is the diffusion of species j.
In the present case standard k-Є model is used due to its suitability for a wide range of wall-bound and free shear flows[5].

3.2 Combustion Model

The global reaction mechanism is modelled to involve the following chemical species: C, O_2, CO, CO_2, H_2O and H_2. All of the species are assumed to mix in the molecular level. [6] The chemical reactions inside the gasifier are modeled by calculating the transport and mixing of the chemical species by solving the conservation equations describing convection, diffusion, and reaction of each component species. The generalized transport equations for chemical species are where S represents various above mentioned species:

$$\frac{\partial}{\partial t}(\rho Y_S) + \nabla(\rho \bar{v} Y_S) = -\nabla \bar{J}_S + R_S \text{ ..... (11)}$$

These equations are solved by the Eddy Dissipation model. The assumption in this model is that the chemical reaction is faster than the time scale of the turbulence eddies [5]. Thus, turbulence mixing of species determines the rate of reaction rate. The reaction is assumed to occur instantaneously when the reactants are in contact with each other.

3.3 Mixture Fraction Model

The reaction chemistry in the probability density function (PDF) method for solving turbulent-chemistry interaction is determined using mixture fraction model. The equilibrium model is used and it assumes that the chemistry is rapid enough for chemical equilibrium to always exist at the molecular level [5]. Basing on the simplifying assumptions, the

instantaneous thermo-chemical state of the fluid is related to the mixture fraction f. Species mole fraction is computed based using minimization of Gibbs free energy concept. The mixture fraction f is defined in terms of the atomic mass fraction as:

$$f = \frac{Z_j - Z_{j,ox}}{Z_{j,fuel} - Z_{j,ox}} \quad \text{..... (12)}$$

Where Z_j is the mass fraction for element j. The subscript ox and fuel denote the value at the oxidizer stream inlet and the fuel stream inlet respectively.

4. Properties of Lignite

Lignite is commonly analyzed by two methods. One is ultimate analysis and the other is proximate analysis. In the present case proximate analysis of lignite is been done and data for ultimate analysis are taken in the Non-Premixed combustion model. The various properties used for lignite are tabulated below:

Table 1. Lignite properties

Properties	Value	Unit
Calorific Value	9300	kJ/Kg
Density	700	kg/m^3
Specific Heat	4500	J/kg-K

5. Result and Discussion

The analysis is performed with second order discretization scheme. Nearly 2500 iterations are performed on FLUENT 6.2.16 & the analysis is run for 4 days. Finally the results are obtained in steady state condition using fluent software.

5.1 Temperature, Velocity, Static Pressure and Mass fraction profiles

Particle temperature is influenced by radiative and convective transport, internal conduction, chemical reaction and also most of it by hot wall impact. The temperature is higher at the areas near the throat (refer Figure 2) because it is affected by the flame/torch that is placed at the wall near the throat. Furthermore, these areas are oxidation zone and reduction zone where all the lignite is burnt.

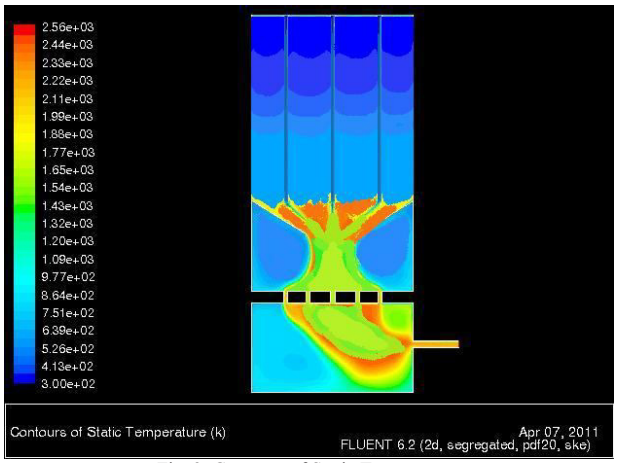

Fig. 2. Contours of Static Temperature

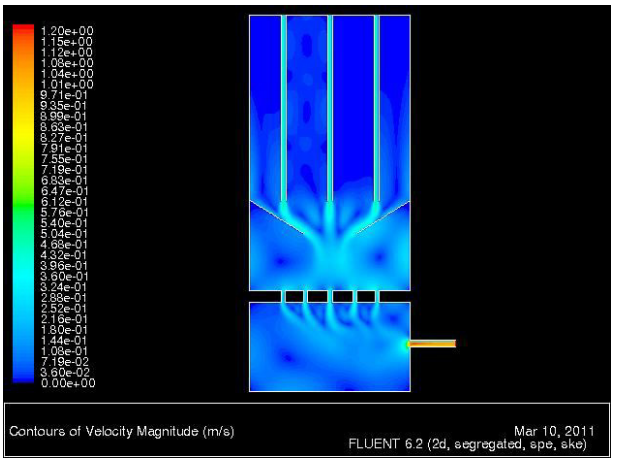

Fig. 3. Contours of Velocity Magnitude

The velocity contours slightly changes near the grate region as well as near the throat region as shown in Figure 3. Whirling phenomenon is achieved when combustion of air is enters throat but when the combustion of coal takes place this phenomenon is vanished. The above value of average velocity is taken when the combustion of coal and air is done.

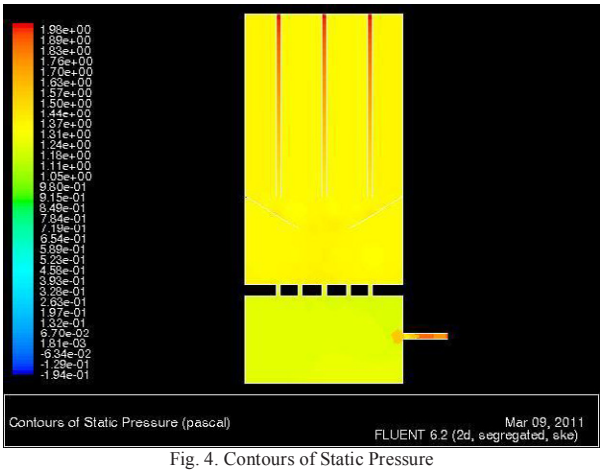

Fig. 4. Contours of Static Pressure

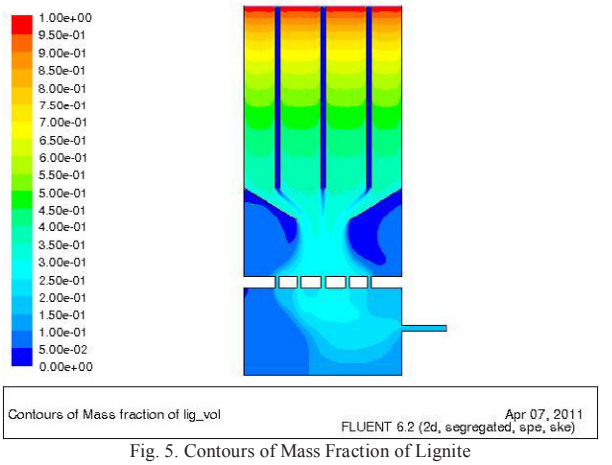

Fig. 5. Contours of Mass Fraction of Lignite

From the contour of static pressure as shown in Figure 4, there is not much different from predicted total pressure. The pressure distributions are roughly the same. The maximum static pressure is 1.98 Pascal and minimum pressure is 1.11 Pascal. There is only a minor change near the grate region and gas outlet nozzle region.

It is seen from the Figure 5 that the particles of lignite are consumed in the combustion process. As the lignite is progressed in downward direction, the mass of lignite is changing. Below the throat region the coal particles are not seen because of the irregular distribution of coal particles. These results did not match with the practical solutions.

5.2 Mass fraction of species

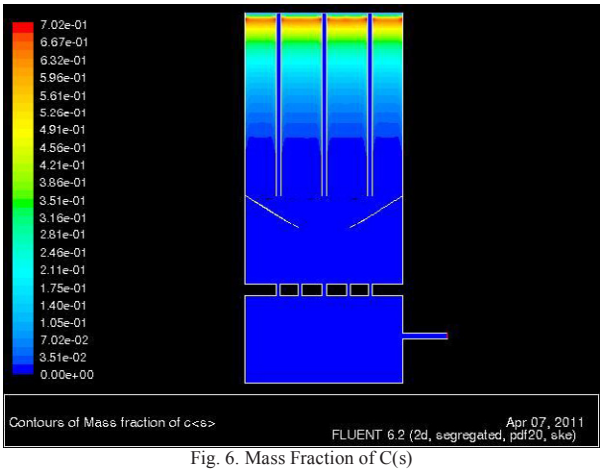

Fig. 6. Mass Fraction of C(s)

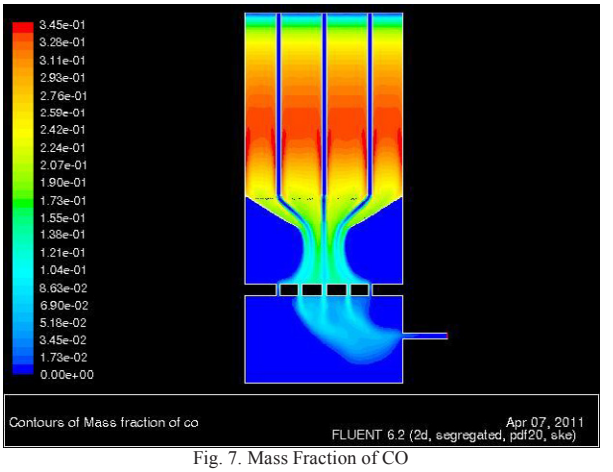

Fig. 7. Mass Fraction of CO

Having the correct gasification kinetics for char is critical for any gasifier model. It is clear from the Figure 6 that as the combustion of coal takes place the char and tar is been made from the coal. But near the throat region, the char-burnout factor is vanished i.e. char is no longer visible in the same region.

It is found from Figure 7 that the mass fraction of CO is well enough in the pyrolysis zone. The amount of CO should vary between 10-30 %.And after the simulation, the average amount of CO is found out to be 20 % which is quite convincing.

From the Figure 8, it is seen that the whole CO_2 is remained only above the grate. The maximum mass fraction of is CO_2 found out to be 23.4 %. The concentration of CO_2 is highest at the exit of the chamber as the gas is going in outward .

The water-Gas shift reaction is in equilibrium throughout most of the reaction chamber. There is some percentage of moisture in the lignite. But as and when the combustion initiates this moisture is vanished simultaneously. In the drying zone, minor portion of the H_2O is observed. But as the combustion is progressed, this H_2O is divided in to H_2 and O_2 molecules. The very high H_2O mass fractions seen in the downstream of the gasifier near the exhaust nozzle.

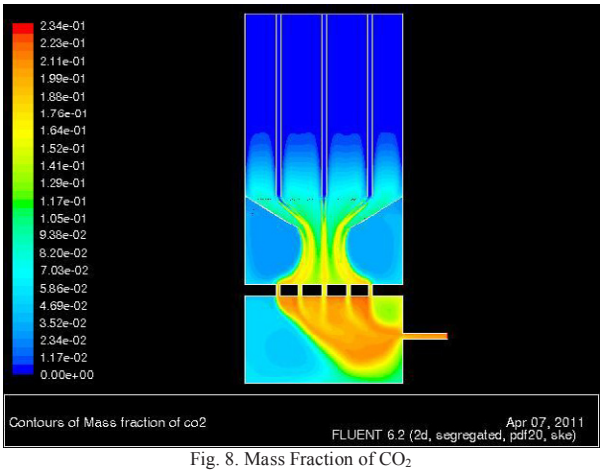

Fig. 8. Mass Fraction of CO_2

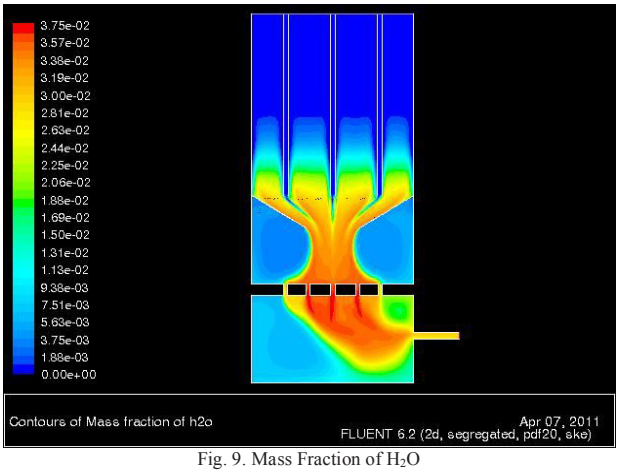

Fig. 9. Mass Fraction of H_2O

The mass fraction of H_2 in this case is 0.023 i.e. 2.3% as shown in Figure 10.This result might be deviated due to the uneven distribution of gas in the reaction chamber.

The reactive O molecules are found out below the grate region as shown in Figure 11. These Oxygen radicals react with the CO and the final outcome from this two is CO_2 which is not desirable. More-or-less the O radicals are converted in to O_2 by heterogeneous reactions which are taking place inside the pyrolysis zone.

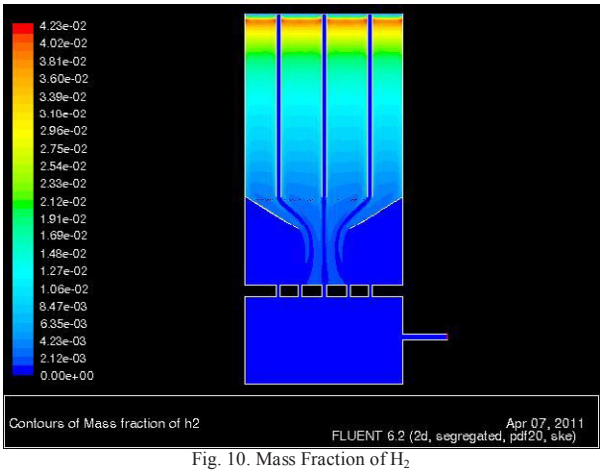

Fig. 10. Mass Fraction of H_2

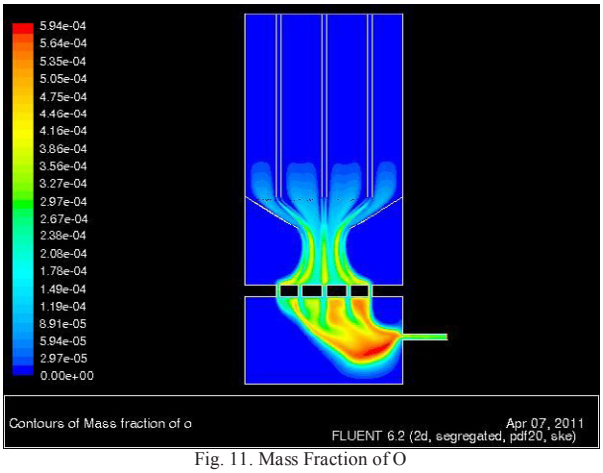

Fig. 11. Mass Fraction of O

6. Conclusions

The model was developed and used to predict the gas composition, reaction temperature, unconverted char and calorific value of gas for known coal composition, initial temperature of pyrolysis zone, velocity of air flow and pressure. Some of the results were found out to be nearer to the experimental results. The validation of the analytical numbers was also done.

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